

The usefulness of energy decomposition schemes to rationalize host-guest interactions

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Abstract

This perspective focuses on the crucial role that energy decomposition schemes play in elucidating the physical nature of non-covalent interactions in supramolecular systems, particularly from the point of view of host-guest systems stabilized by non-covalent interactions, which are fundamental to molecular recognition. The findings reported here reveal the robustness and practical application of methods such as EDA-NOCV in rationalizing molecular recognition situations in systems such as calixarenes, cyclophanes and other box-shaped hosts, capable of incorporating different chemical species as anions and PAHs. We expect that the discussed cases in this perspective can be viewed as an initial assessment for the multidimensional nature of the weak interactions underlying supramolecular aggregations, which can be recognized in a plethora of different structures constantly synthesized and characterized by chemists around the world. This journal is